Study of Alloy Induced Disorder in Quantum Dots using Tight-binding

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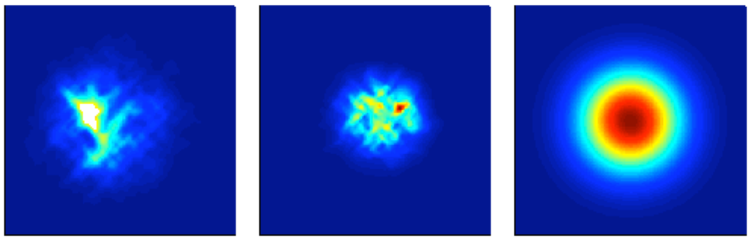
The "standard" method for computing electronic structure of quantum dots is **k.p**. However, this jellium-like model is fundamentally not well suited for the atomistic representation of nanoscale features. It has been demonstrated that the envelope function approximation central to **k.p** degrades as the minimum feature size approaches the length of several monolayers or less. Two principal approaches, tight-binding and pseudopotential methods, are typically used to model solids on finer length scales. We have pursued the tight-binding approach for our ability to leverage previous Nanoelectronic Modeling (NEMO) developments. Our simulation employs a nearest-neighbor empirical tight-binding method $sp^3d^5s^*$ with a 20 orbital basis, consisting of s, p, and d orbitals, associated with each atomic lattice site. Since the basis set that is used is not complete in a mathematical sense, the parameters that enter the model are determined by a fit to experimental data, and a genetic algorithm package is used to determine a set of orbital couplings that reproduces a large number of physical observables of the bulk binary system, including bandgaps and effective masses at various symmetry points in the Brillouin zone. Because the orbital couplings also depend on the relative positions of the nearest neighbor atoms, an accurate calculation of the electronic structure requires an accurate representation of the positions of each atom. NEMO-3D uses a valence force field (VFF) model to minimize the total strain energy, expressed as a sum of local (nearest-neighbor) functionals of atomic positions.

In this work we examine the issue of alloy-induced disorder, particularly as it applies to linewidth broadening. That is, given an ensemble of quantum dots with identical alloy composition, we explore the fundamental limits of linewidth broadening that arise solely as a result of variations in configurations of cations in the quantum dots and ignore any additional contributions such as size variation, strain-induced spatial perturbations on a QD due to neighboring QDs, and many-body effects. It is found that alloy-induced broadening is small (~0.35 meV) relative to the observed inhomogeneous broadening obtained from photoluminescence measurements (~20 meV), but comparable to the linewidth broadening found for individual quantum dots at low temperature (~0.5 meV). The resulting calculations show that although the variation in eigenenergies may be fairly small, disordered systems can produce large local variations in the ground state wave function. Figure (1) shows the ground state hole wave function for two different random configurations of a dome-shaped $In_{0.6}Ga_{0.4}As$ quantum dot of diameter 30nm and height 5.4 nm embedded in bulk GaAs and also for an artificial material of the same dimensions whose parameters are determined from the virtual crystal approximation (right). Finally, details of the numerical implementation will be presented. It is demonstrated that convergence of the strain calculation is the principal limiting factor in the overall convergence of the eigenenergies.



The two left figures are isosurface slices through the center of ground state hole wavefunctions for two different random configurations of an $In_{0.6}Ga_{0.4}As$ QD. The right-most figure assumes a uniform VCA material. The height and width of each subfigure is 24 nm.